

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.52

Global applicability domain: Inside

Local applicability domain index: 5.33e-01

Confidence level: 5.40e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Didemethylchlorpromazine</div> <div>Measured: 4.47</div> <div>Predicted: 3.37</div>	<div>Image not found</div> <div>Pyrifenox</div> <div>Measured: 3.70</div> <div>Predicted: 3.80</div>
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